Studies of electron correlations in lithium

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INTRODUCTION

The electronic structure of lithium as one of the simplest atomic systems has stimulated great experimental and theoretical interest[1,2]. Comparison of experimental data with *ab initio* calculations on Li ground, excited and ionic states sheds light onto fundamental questions of electron correlation phenomena and advances theoretical models for more complex systems. We performed high-resolution electron spectroscopy of *1snl* satellites in Li *1s* photoionization, resolving the LS term structure for the $n>2$ lines for the first time. Experimental branching ratios are compared with R-matrix calculations.

EXPERIMENT

The experiment was carried out at the Atomic and Molecular undulator beamline 10.0.1 of the ALS. The electron spectra were measured using an end station designed for gas-phase angle-resolved studies and based on the Scienta SES-200 hemispherical analyzer. The analyzer is rotatable in a plane perpendicular to the propagation direction of the beam of linearly polarized photons allowing electron angular distribution studies. A resistively heated metal vapor oven was used to generate an effusive beam of Li atoms, intersecting the photon beam.

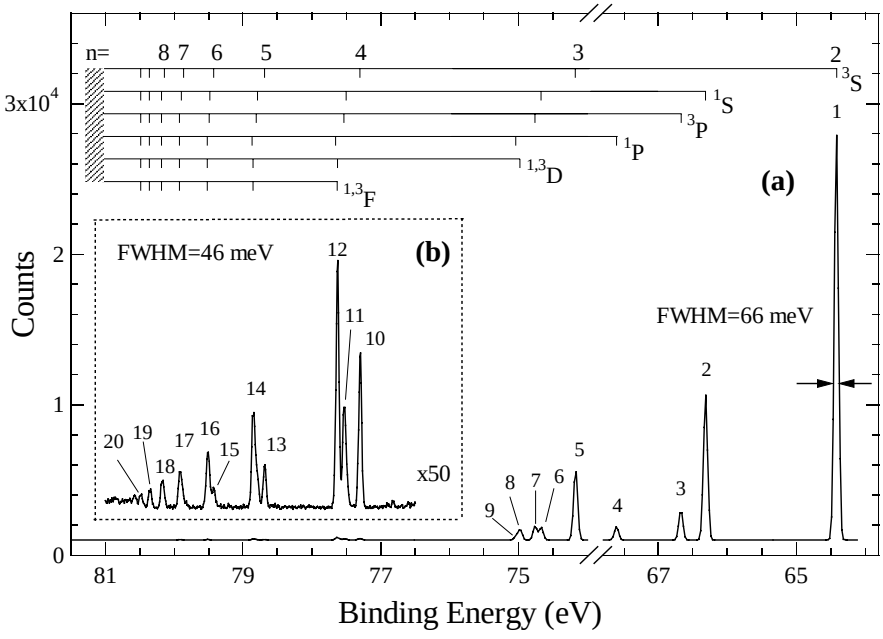

Figure 1. Photoelectron spectrum of the Li^+ *1snl* satellites taken at 100 eV photon energy.

RESULTS

Li *1s* photoelectron spectrum with the 1snl satellites is shown in Fig. 1. The regions of the *1s3l* and *1s4l* satellite lines were also measured with higher (37 meV FWHM) experimental resolution. Branching ratios were extracted from spectra similar to Fig. 1. For the 1s2l group, our results show a good agreement with previous measurements[2]. For *1snl*, *n*>2, no published experimental data exists. The branching ratios of the lines within the *1s3l* group are compared with 19-state basis R-matrix calculations in Fig.2. Similar comparison was made for the *1s4l* group and some of the tendencies were also studied in higher-n groups for which the term structure is less resolved.

The experimental results and R-matrix calculations agree well in the case of the ^{1}S and ^{1}P ratios to the ^{3}S line. For the ^{3}P line and for the lines with higher angular momentum (^{1,3}D,F), the calculations represent qualitatively the energy dependeny of the branching ratios, but over- or underestimate the absolute values of the cross-sections.

Studying the photon energy dependency of the terms with different angular momentum allows one to draw conclusions about the principal mechanisms responsible for these transitions. Of particular interest is the ratio of the D and F terms to the P-lines. The present spectra provide conclusive evidence that this ratio is energy-independent over the studied energy range for the *1s3l* and *1s4l* groups. Also for the *1s5l* and *1s6l* groups, the D,F-to-P ratio shows no energy dependency beyond the error bars. In contrast, the ratios of the lines with L>0 terms to the ^{1,3}S lines decrease rapidly with photon energy. This behavior strongly suggests that different mechanisms are producing the S-terms and the higher-L terms. The traditional shake-up model based on electron relaxation seems to describe well the S-terms, whereas the higher-L terms are created mainly by electron collision ("knock-out") processes, involving the departing *1s* electron and the *2s* valence electron.

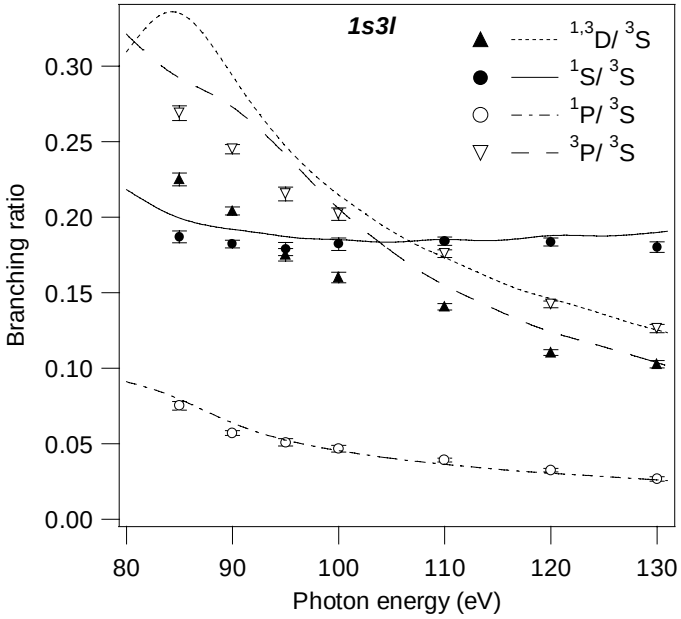

Figure 2. Branching ratios of the lines in the *1s3l* satellite group. R-matrix calculations are shown by lines.

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